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## ABSTRACT

In the first part of the paper cross sections for the electron impact ionization of the  $2s$  and the  $2p$ ,  $m = 0, \pm 1$  states of atomic hydrogen have been calculated, using two forms, B.E. (i) and B.E. (ii), of the Born exchange approximation. For the form B.E. (i) it is found that inclusion of exchange increases the cross section for the  $2p_{m = \pm 1} \rightarrow c$  transition but decreases the cross sections for the  $2s \rightarrow c$  and  $2p_{m = 0} \rightarrow c$  transitions. In the B.E. (ii) calculation inclusion of exchange necessarily decreases the cross sections. For the  $2s \rightarrow c$  transition Prasad's Born exchange calculations are verified.

In the second part the binary collision approximation of Vainshtein has been applied to the  $2s$  and the  $2p$  ionization and it is found that the Vainshtein approximation with its proper choice of effective charge does not agree with the Born exchange approximation. A new expression for the exchange amplitude has been derived in the Vainshtein approximation.

We have concluded by comparing the results of the Born, the Born exchange, the Born-Ochkur, and the Vainshtein's approximation for the ionization of the  $1s$ ,  $2s$  and the  $2p$  states of atomic hydrogen.

## I. INTRODUCTION

In this paper<sup>1</sup> the impact ionization cross sections for the second quantum level of atomic hydrogen are calculated by two different procedures. The first is the Born exchange approximation developed by Peterkop.<sup>2</sup> This method has been studied and applied to the ionization of H(1s) and H(2s) by several authors.<sup>3-7</sup> However for the 2p states, because of the mathematical complexity, the Born exchange calculation has not been so far carried out. This will be done in Sec. II.

We have also calculated these cross sections using both the original binary collision approximation of Vainshtein et al.,<sup>8,9</sup> and the modified form developed by Omidvar<sup>10</sup> and Crothers.<sup>11</sup> In this case the two forms of the binary collision theory yield cross sections which can differ by as much as an order of magnitude. In Sec. III we formulate the theory and point out the approximations which have been made. Vainshtein et al. included exchange by an approximation similar to that used by Ochkur.<sup>12</sup> It is shown in Sec. III that the exchange term can be treated by the same type of procedure used to solve the direct matrix element.<sup>13</sup>

In Sec. IV the results of our calculations are presented and compared with Born and Born Ochkur calculations.

## II. BORN EXCHANGE

### A. General Theory

If we let  $\mathbf{k}_1$ ,  $\mathbf{k}_2$  and  $\mathbf{k}$  represent respectively the momenta of the incident, scattered and ejected electrons, the total cross section for the ionization of atomic hydrogen by electron impact is given in atomic units by

$$Q = \frac{1}{4\pi^2 k_1} \int_0^{\epsilon/2} k_2 k d\epsilon \int \left\{ \frac{3}{4} |T - T_{\text{ex}}|^2 + \frac{1}{4} |T + T_{\text{ex}}|^2 \right\} d\hat{\mathbf{k}} d\hat{\mathbf{k}}_2. \quad (1)$$

Here  $\epsilon$  is the energy of the ejected electron in atomic units,  $\epsilon =$  the maximum value of  $\epsilon$ , and  $\hat{\mathbf{k}}$  and  $\hat{\mathbf{k}}_2$  represent unit vectors in the directions of  $\mathbf{k}$  and  $\mathbf{k}_2$  respectively. For transitions from atomic state 1 to state 2 the direct amplitude,  $T(1,2)$ , and the exchange amplitude,  $T_{\text{ex}}(1,2)$  are given by

$$T(1, 2) = \langle \varphi_2(\mathbf{r}_1) e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| \psi(\mathbf{r}_1, \mathbf{r}_2) \rangle, \quad (2)$$

$$T_{\text{ex}}(1, 2) = \langle \varphi_2(\mathbf{r}_2) e^{i\mathbf{k}_2 \cdot \mathbf{r}_1} \left| \frac{1}{r_{12}} - \frac{1}{r_1} \right| \psi(\mathbf{r}_1, \mathbf{r}_2) \rangle, \quad (3)$$

where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the coordinates of the atomic and incident electrons with respect to an infinitely heavy nucleus,  $\psi(\mathbf{r}_1, \mathbf{r}_2)$  is the total wave function, and  $\varphi_2(\mathbf{r})$  is the final atomic state.

If we are dealing with ionization the matrix elements (2) and (3) can be reduced to functions of  $\mathbf{k}$  and  $\mathbf{k}_2$ , hence in this paper we will often write the transition amplitudes in the form  $T(\mathbf{k}, \mathbf{k}_2)$  and  $T_{\text{ex}}(\mathbf{k}, \mathbf{k}_2)$ .

Peterkop<sup>2</sup> showed that the exchange matrix element  $T_{\text{ex}}(\mathbf{k}, \mathbf{k}_2)$  could be derived from the direct matrix element  $T(\mathbf{k}, \mathbf{k}_2)$  by interchanging the wave vectors  $\mathbf{k}$  and  $\mathbf{k}_2$  of the ejected and scattered electrons and multiplying the resultant by a phase factor. That is

$$T_{\text{ex}}(\mathbf{k}, \mathbf{k}_2) = e^{i\delta(\mathbf{k}, \mathbf{k}_2)} T(\mathbf{k}_2, \mathbf{k}). \quad (4)$$

He was not, however, able to specify an unambiguous method of calculating  $\delta(\mathbf{k}, \mathbf{k}_2)$ . Later Peterkop<sup>3</sup> used the first Born approximation to study the contribution of exchange to the cross section for the ground state ionization of hydrogen atom by incident electrons. He chose

$$\delta(\mathbf{k}, \mathbf{k}_2) = 0 \quad (5)$$

as a reasonable value, but he also considered the case

$$\delta(\mathbf{k}, \mathbf{k}_2) = \arg T(\mathbf{k}, \mathbf{k}_2) - \arg T(\mathbf{k}_2, \mathbf{k}) \quad (6)$$

This latter case yields the maximum interference between the direct and exchange amplitudes and hence the minimum cross section. Prasad<sup>4</sup> duplicated Peterkop's ground state calculation and also applied the theory to H(2s). Other phase choices have been suggested by Rudge and Seaton<sup>5</sup> who have carefully studied this problem. We will, however, here consider only the two choices given above. These choices will be hereafter also be designated as B.E. (i) and B.E. (ii) for Eq. (5) and (Eq. (6) respectively.

For comparison purposes we also calculate the cross sections in the Born-Ochkur exchange approximation in which one retains only the first term of the

expansion of  $T_{\text{ex}}(1,2)$  in reciprocal powers of  $k_1$ . In the ionization case the exact first term is not normally used. Several simplified versions of this approximation have been published. We here use that of Prasad<sup>4</sup> who put

$$T_{\text{ex}}(1,2) = \left( \frac{q}{k_1} \right)^2 T^{\text{B}}(1,2), \quad (7)$$

where  $q = k_1 - k_2$ , and  $T^{\text{B}}(1,2)$  is the Born transition amplitude. This differs slightly from the equation given by Ochkur<sup>12</sup> for ionization but yields similar cross sections.

### B. Calculation of the Exchange Cross Sections

Let  $\ell$  and  $m$  be respectively the angular momentum and magnetic quantum numbers of the atomic electron, and let the  $z$  axis of the system be along the momentum transfer vector  $q = k_1 - k_2$ . In the Born approximation the transition amplitude for the ionization of  $H(2, \ell, m)$  can then be written<sup>14</sup>

$$T(\mathbf{k}, \mathbf{k}_2) = \frac{ABCe^{im\beta'} [(M_0 + iN_0) + (M_1 + iN_1)(\hat{\mathbf{q}} \cdot \hat{\mathbf{k}}) + (M_1 + iN_2)(\hat{\mathbf{q}} \cdot \hat{\mathbf{k}})^2]}{\gamma^{3+i\alpha_0} D^\lambda} \quad (8)$$

where

$$\alpha_0 = \frac{1}{k}, \quad B = \frac{1}{q} \left( \frac{2\pi\alpha_0}{1 - \exp(-2\pi\alpha_0)} \right)^{1/2},$$

$$\gamma = \frac{\frac{1}{4} + (q - k)^2}{\left( \frac{1}{2} + ik \right)^2 + q^2}, \quad D = \frac{1}{4} \left[ \left( \frac{1}{2} + ik \right)^2 + q^2 \right]. \quad (9)$$

And  $\beta'$  is the azimuthal angle of  $\mathbf{k}$  in the coordinate system  $(x', y', z')$ , (Cf. Fig. 1), which has  $\mathbf{q}$  as its polar axis.



The quantities  $A$ ,  $C, \lambda$ ,  $M_i$  and  $N_i$  are dependent on the quantum numbers  $\ell$  and  $m$ . They are:

2s case: ( $\ell = 0$ ,  $m = 0$ )

$$A = \frac{1}{256} ; \quad C = 1, \lambda = 5$$

$$M_0 = q \left[ \frac{1}{8} - 2k^2 - 3q^2 - 2k^4 + 2q^4 \right],$$

$$M_1 = -k \left[ \frac{7}{8} - k^2 - 7q^2 - 2k^4 - 4k^2 q^2 + 6q^4 \right],$$

$$M_2 = q [1 - 3k^2 - 4k^4 + 4k^2 q^2],$$

$$N_0 = qk,$$

$$N_1 = - \left[ -\frac{1}{8} + 2k^2 + 3q^2 + 2k^4 - 2q^4 \right],$$

$$N_2 = (4qk) (1 + k^2 - q^2). \quad (10)$$

2p m = 0 case: ( $\ell = 1$ ,  $m = 0$ )

$$A = \frac{1}{256} ; \quad C = 1; \lambda = 5$$

$$M_0 = k \left( \frac{1}{4} + k^2 + 3q^2 \right)$$

$$N_0 = - \left( \frac{1}{16} + \frac{3}{2} q^2 - k^4 - 3q^4 \right)$$

$$M_1 = q (1 - 4k^2 - 4q^2)$$

$$N_1 = kq (4 - 8q^2)$$

$$M_2 = k \left( -\frac{5}{4} - k^2 + 5q^2 \right)$$

$$N_2 = \left( \frac{1}{4} - \frac{3}{2} k^2 - q^2 - 2k^4 + 6k^2 q^2 \right) \quad (11)$$

2p m = ±1 case: ( $\ell = 1$ ,  $m = \pm 1$ )

$$A = \frac{1}{32\sqrt{2}}; \quad C = (1 - ik) [1 - (\hat{\mathbf{q}} \cdot \hat{\mathbf{k}})]^{1/2}; \quad \lambda = 4$$

$$\begin{aligned} M_0 &= q & N_0 &= 0 \\ M_1 &= -k & N_1 &= \frac{1}{2} \\ M_1 &= 0 & N_2 &= 0. \end{aligned} \tag{12}$$

The exchange matrix element (4), with phase choice (5) or (6) is found by interchanging  $\mathbf{k}$  and  $\mathbf{k}_2$  in Eqs. (8) to (12). But in the exchange matrix element the polar axis is  $\mathbf{q}_{\text{ex}} = \mathbf{k}_1 - \mathbf{k}$ . Both  $\mathbf{q}$  and  $\mathbf{q}_{\text{ex}}$  must be referred to a common coordinate system if we are to evaluate the interference integral,

$$Q^{\text{int}} = \frac{1}{4\pi^2 k_1} \int_0^{\epsilon/2} k k_2 d\epsilon \int \text{Re} [T(\mathbf{k}, \mathbf{k}_2) T_{\text{ex}}^*(\mathbf{k}, \mathbf{k}_2)] d\hat{\mathbf{k}} d\hat{\mathbf{k}}_2, \tag{13}$$

which occurs in (1). As illustrated in Fig. 1, we choose (x,y,z) as our fixed reference system with  $\hat{\mathbf{z}} = \hat{\mathbf{k}}_1$ . The polar and azimuthal angles of  $\mathbf{k}$  and  $\mathbf{k}_2$  are respectively ( $\alpha, \beta$ ) and ( $a, b$ ) in the (x,y,z) system, and ( $\alpha', \beta'$ ) and ( $a', b'$ ) in the (x', y', z') system. Since the position of x' in the (x', y') plane is arbitrary, we choose  $\mathbf{x}' \perp \mathbf{k}_1$  so that only two Eulerian angles,  $\Theta$  and  $\Phi$  are required to describe the transformation from the unprimed to the primed systems. Now all of the quantities appearing in direct and exchange matrix elements are scalars and invariant under rotation of the coordinate system except the terms containing the azimuthal angles  $\beta'$  and  $\beta'_{\text{ex}}$  which refer to two different coordinate systems. The necessary transforms for these two angles are given by<sup>15</sup>

$$\tan \beta' = \frac{\text{ctn } \alpha \sin \Theta}{\sin (b - \beta)} + \cos \Theta \text{ctn } (b - \beta),$$

$$\cos \Theta = \mathbf{q} \cdot \mathbf{k}_1 / qk_1. \quad (14)$$

Equation (14) is similarly used for the transformation of  $\beta'_{\text{ex}}$  if  $\mathbf{k}$  and  $\mathbf{k}_2$  are interchanged.

It can be shown that in the five dimensional integral in (1) the azimuthal variables  $\beta$  and  $b$  appear only in the form  $(b - \beta)$ , and this allows one of them to be analytically integrated. The four remaining integrations were performed numerically by Gaussian Quadrature. The numerical results are presented and discussed in Sec. IV.

### III. THE VAINSHTEIN APPROXIMATION

#### A. Theory

In this theory, qualitatively speaking, the problem is considered as a binary collision between the incident and atomic electrons in the Coulomb field of an infinitely heavy nucleus. This approximation was introduced by Vainshtein et al.,<sup>8</sup> with the hope that it would give a marked improvement over the more usual procedure of treating the interelectronic interaction as a perturbation. In some cases it appears to have done so, but recently the validity of the three approximations made in the theory has been questioned.<sup>10,16</sup> These three are (a) the effective charge approximation; (b) the peaking approximation and (c) the change in sign of an exponential argument. Below we formulate the theory, but some

details previously given by Vainshtein et al., are omitted. On the other hand the derivation of the effective charge has not been given by Vainshtein et al. For the benefit of the reader who is not familiar with the method, this derivation will be given in Appendix A, and it is shown that the approximation of the effective charge is subject to many questions. We then apply the method to the ionization of hydrogen atoms in its first excited states. The results indicate that there is need for further investigation of this theory.

The exact wave function is written in the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \varphi_1(\mathbf{r}_1) g(\mathbf{r}_1, \mathbf{r}_2), \quad (15)$$

where  $\varphi_1(\mathbf{r})$  is the initial atomic state and  $g(\mathbf{r}_1, \mathbf{r}_2)$  a function which will be derived below. If this is substituted into the Schrödinger equation and the new variables  $\mathbf{R} = (\mathbf{r}_2 + \mathbf{r}_1)/2$  and  $\boldsymbol{\rho} = (\mathbf{r}_2 - \mathbf{r}_1)/2$  are introduced then

$$\begin{aligned} (1/2 \nabla_{\mathbf{R}}^2 + 1/2 \nabla_{\boldsymbol{\rho}}^2 + \zeta/R - \zeta/\rho + k_1^2) g(\mathbf{R}, \boldsymbol{\rho}) &= Q g(\mathbf{R}, \boldsymbol{\rho}), \\ Q &= \zeta/R - 2/|\mathbf{R} + \boldsymbol{\rho}| + (1 - \zeta)/\rho \\ &\quad - (\nabla_1 \ln \varphi_1) \cdot (\nabla_{\mathbf{R}} \ln \chi - \nabla_{\boldsymbol{\rho}} \ln \chi), \\ \chi &= e^{-i\mathbf{k}_1 \cdot (\mathbf{R} + \boldsymbol{\rho})} g(\mathbf{R}, \boldsymbol{\rho}). \end{aligned} \quad (16)$$

The solution of the homogeneous equation,  $Q = 0$ , with the correct asymptotic form is

$$\begin{aligned} g_0(\mathbf{R}, \boldsymbol{\rho}) &= N e^{i\mathbf{k}_1 \cdot (\mathbf{R} + \boldsymbol{\rho})} F(i\nu, 1, i\mathbf{k}_1 \cdot \mathbf{R} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}) \\ &\quad \times F(-i\nu, 1, i\mathbf{k}_1 \cdot \boldsymbol{\rho} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}). \end{aligned} \quad (17)$$

where  $N = \Gamma(1 - i\nu) \Gamma(1 + i\nu)$  and  $\nu = \zeta/k_1$ . We will use an effective charge,  $\zeta$ , which was derived by Vainshtein et al. and which tends to minimize  $Q$  when  $\rho$  and  $R$  are large:

$$\zeta = \frac{k_1}{k_1 + \sqrt{2\epsilon_1}}, \quad (18)$$

$\epsilon_1$  being the ionization potential of the initial state of the target atom.

The use of the homogeneous solution (17) together with (18) is known as the effective charge approximation. The cross sections obtained by this method are moderately sensitive to the choice of  $\zeta$ .

In evaluating the direct matrix element  $T(1,2)$  Vainshtein et al. dropped the core term  $1/r_2$  from the interaction potential  $(1/r_{12} - 1/r_2)$ , since it gives a zero contribution to the transition amplitude in the Born approximation. This is probably not justified in their theory since their initial and final wave functions are not orthogonal. In Appendix B this term has been treated and it is found that the peaking approximation is not applicable. To simplify the problem we therefore also neglect the core term, substitute (15) and (17) in (2), apply the peaking approximation and obtain

$$T(1, 2) = \frac{4\pi}{q^2} A \langle \varphi_2 | e^{i\mathbf{q} \cdot \mathbf{r}} | \varphi_1 \rangle \quad (19)$$

where

$$A = \frac{Nq^2}{\pi} \lim_{\lambda \rightarrow 0} \int \frac{e^{2i\mathbf{q} \cdot \boldsymbol{\rho} - \lambda \rho}}{\rho} F(i\nu, 1, i\mathbf{k}_1 \cdot \boldsymbol{\rho} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}) \\ \times F(-i\nu, 1, i\mathbf{k}_1 \cdot \boldsymbol{\rho} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}) d^3 \rho. \quad (20)$$

Vainshtein et al. put (20) in the form of Nordsieck's Integral<sup>17</sup> by changing  $e^{2i\mathbf{q} \cdot \mathbf{p}}$  to  $e^{-2i\mathbf{q} \cdot \mathbf{p}}$  and obtained

$$T(1, 2) = \frac{4N\pi}{q^2} \tilde{\varphi}(\mathbf{q}) F(-i\nu, i\nu, 1, x),$$

$$x = \left( \frac{\Delta\epsilon + q^2}{\Delta\epsilon + 3q^2} \right)^2, \quad \Delta\epsilon = k_1^2 - k_2^2. \quad (21)$$

Here the Fourier transform  $\tilde{\varphi}(\mathbf{q})$  is defined by

$$\tilde{\varphi}(\mathbf{q}) = \left( \frac{1}{2\pi} \right)^3 \langle \varphi_2(\mathbf{r}) | e^{i\mathbf{q} \cdot \mathbf{r}} | \varphi_1(\mathbf{r}) \rangle.$$

Notice from (21) that the ratio of  $T(1, 2)$  to  $T^B(1, 2)$  is given by

$$F(i\nu, -i\nu, 1; X)/F(i\nu, -i\nu, 1; 1)$$

which for  $X < 1$  is always less than unity. Thus the effect of the change of sign is to make the cross section calculated by Vainshtein's method always less than the Born cross section.

Omidvar<sup>10</sup> and Crothers<sup>11</sup> have pointed out that the integral in (20) can be evaluated exactly. They obtained:

$$A = \frac{\Gamma(1 + i\nu) \Gamma(-2i\nu)}{\Gamma(-i\nu)} e^{(\mp)\pi\nu} e^{-i\nu \ln y} F(i\nu, i\nu, 1 + 2i\nu, 1/y)$$

$$+ \frac{\Gamma(1 - i\nu) \Gamma(2i\nu)}{\Gamma(i\nu)} e^{(\pm)\pi\nu} e^{i\nu \ln y} F(-i\nu, -i\nu, 1 - 2i\nu, 1/y),$$

$$y = \left( \frac{q^2 + \Delta\epsilon}{q^2 - \Delta\epsilon} \right). \quad (22)$$

In  $e^{(\mp)\pi\nu}$  the top sign is to be taken if  $q^2 > \Delta\epsilon$  and the bottom sign if  $q^2 < \Delta\epsilon$ .

## B. Exchange

Vainshtein et al. included exchange in their theory by an approximation which has similarities to the Born-Ochkur approximation. This approximation leads to the Born-Ochkur exchange formula if the function  $g(\mathbf{r}_1, \mathbf{r}_2)$  in (15) is replaced by  $e^{i\mathbf{k}_1 \cdot \mathbf{r}_2}$ . Their equation for the exchange amplitude is

$$T_{\text{ex}}(1, 2) = \frac{4N\pi}{q^2} \tilde{\varphi}(\mathbf{q}) F\left(-i\nu, i\nu, 1, \frac{1}{4}\right). \quad (23)$$

We will proceed to evaluate the exchange amplitude in the same framework as the direct amplitude was evaluated, and we avoid the additional approximation used by Vainshtein for the evaluation of exchange. The final result has previously been reported.<sup>13</sup> It is helpful in this case to introduce Fourier transforms  $\tilde{\varphi}_1(\mathbf{p}_1)$  and  $\tilde{\varphi}_2(\mathbf{p}_2)$  for  $\varphi_1(\mathbf{r}_1)$  and  $\varphi_2(\mathbf{r}_2)$  respectively. As before we make the peaking approximation and carry out the  $\mathbf{R}$  integral to obtain for the electron-electron interaction term

$$\begin{aligned} T_{\text{ex}}^e(1, 2) &= \langle \varphi_2(\mathbf{r}_2) e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} \left| \frac{1}{r_{12}} \right| \psi(\mathbf{r}_1, \mathbf{r}_2) \rangle \\ &= \frac{N}{2} \lim_{\lambda \rightarrow 0} \int \tilde{\varphi}_1\left(\frac{\mathbf{t} - \mathbf{q}}{2}\right) \tilde{\varphi}_2^*\left(\frac{\mathbf{t} + \mathbf{q}}{2}\right) d^3 t \\ &\quad \times \int \frac{e^{i(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{t}) \cdot \boldsymbol{\rho} - \lambda \rho}}{\rho} F(-i\nu, 1, i\mathbf{k}_1 \cdot \boldsymbol{\rho} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}) d^3 \rho. \end{aligned} \quad (24)$$

Before performing the  $\boldsymbol{\rho}$  integral it is helpful to introduce  $\boldsymbol{\tau} = (\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{t})/2$ .

We then obtain

$$T_{\text{ex}}^e(1, 2) = 4N \int \tilde{\varphi}_1(\mathbf{k}_2 - \boldsymbol{\tau}) \tilde{\varphi}_2^*(\mathbf{k}_1 - \boldsymbol{\tau}) I(\boldsymbol{\tau}) d^3\boldsymbol{\tau} \quad (25)$$

where

$$I(\boldsymbol{\tau}) = \lim_{\lambda \rightarrow 0} \frac{4\pi}{(\lambda^2 + 4\tau^2)} \left\{ \frac{\lambda^2 + 4\tau^2}{\lambda^2 + 4\tau^2 - 4\mathbf{k}_1 \cdot \boldsymbol{\tau} - 2i\mathbf{k}_1 \lambda} \right\}^{-i\nu}$$

$$= \frac{\pi}{\tau^2} e^{i\nu \ln\{|\tau^2 - \mathbf{k}_1 \cdot \boldsymbol{\tau}|/\tau^2\} + \nu\varphi}, \quad (26)$$

$$\varphi = 0 \text{ if } \tau^2 - \mathbf{k}_1 \cdot \boldsymbol{\tau} > 0$$

$$= \pi \text{ if } \tau^2 - \mathbf{k}_1 \cdot \boldsymbol{\tau} < 0.$$

In (26) the azimuthal integral can be carried out analytically, but the polar and radial integrals must be done numerically. However in the case of ionization  $\tilde{\varphi}_2^*(\mathbf{k}_1 - \boldsymbol{\tau})$ , the Fourier transform of the Coulomb wave function, contains a third order pole at  $\mathbf{k}_1 - \mathbf{k} - \boldsymbol{\tau} = 0$ . In the usual fashion we can therefore use the peaking approximation to remove  $I(\mathbf{k}_1 - \boldsymbol{\tau})$  from under the integral sign. It can then be shown that

$$\int \tilde{\varphi}_1(\mathbf{k}_2 - \boldsymbol{\tau}) \tilde{\varphi}_2^*(\mathbf{k}_1 - \boldsymbol{\tau}) d^3\boldsymbol{\tau}$$

$$= \int \varphi_2^*(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} \varphi_1(\mathbf{r}) d^3\mathbf{r} = \frac{q^2}{4\pi} T^B(1, 2). \quad (27)$$

Hence

$$T_{\text{ex}}^e(1, 2) = q^2 N T^B(1, 2) \text{Exp} \{ \nu\varphi_1 + i\nu \ln[|k^2 - \mathbf{k} \cdot \mathbf{k}_1|/(\mathbf{k}_1 - \mathbf{k})^2] \},$$

$$\varphi_1 = 0 \text{ if } k^2 - \mathbf{k} \cdot \mathbf{k}_1 > 0$$

$$= \pi \text{ if } k^2 - \mathbf{k} \cdot \mathbf{k}_1 < 0. \quad (28)$$



In this approximation the core potential term can be evaluated. The integrals are similar to those in the direct core term, Appendix B. With the aid of the usual peaking approximation we find

$$T_{\text{ex}}^c(1, 2) = - \langle \varphi(\mathbf{r}_2) e^{i\mathbf{k}_2 \cdot \mathbf{r}_1} \left| \frac{1}{r_1} \right| \psi(\mathbf{r}_1, \mathbf{r}_2) \rangle$$

$$\cong - (2\pi)^3 N X_1(\mathbf{k}_2) \varphi_2^*(\mathbf{k}_1). \quad (29)$$

Here  $X_1(\mathbf{p})$  is the Fourier transform of  $\varphi_1(\mathbf{r})/r$ . It has been pointed out<sup>13</sup> that in this approximation the value of  $T_{\text{ex}}^c(1, 2)$  is unchanged if the core potential is taken to be  $1/r_2$  instead of  $1/r_1$ .

#### IV. RESULTS AND DISCUSSION

##### A. Numerical Accuracy

Each four dimensional numerical quadrature in the Born exchange calculation, Sec. II, consumed many minutes of computer time. It was not therefore always practical to check the accuracy of the integrals by doubling the number of points in each quadrature. The accuracy of our results was checked both by examining the convergence of the integrals as the number of Gaussian points used was increased and by comparison with the (2s) results of Prasad<sup>4</sup> and with the Born cross sections.<sup>18</sup> The number of Gaussian points needed to obtain convergence to four significant figures increases as the energy of the incident electron increases. At an incident energy of 1.44 Ryd. we used 40 points in each of the angular integrations and 10 points in the energy quadrature. Because

of the time restrictions on the availability of the computer we used these same number of points at 3.24 Rydbergs. However, our results at this energy may be as much as 1% too small; we therefore did not run any higher energies. Our first Born cross sections are within .2% or better of Omidvar's 1965 results at 1.44 Ryd. and below except at .36 Ryd. where we differ by as much as .6%. In the (2s) case we generally agree with Prasad (1965) to within 1% or better. However, at 0.64 Ryd. his B.E. (i) cross section is 9% lower than ours. We wonder if this may not be due to a clerical error on his part.

Shown in Table 1 are the first Born and the Born exchange cross sections B.E. (i) and B.E. (ii) calculated by four dimensional numerical quadrature. Recall that B.E. (ii), Eq. (6), corresponds to the maximum possible interference and therefore to the minimum cross section in this approximation.

#### B. Effect of the Vainshtein approximations

The no exchange binary collision approximation cross sections for the ionization of H(1s), H(2s) and H(2p) by electron impact are given in Figs. 2-4. Curves 1A and 1B were calculated using the Vainshtein et al., transition amplitude (21), while curves 2A and 2B represent the present theory (19) and (22). A refers to an effective charge of unity (no screening by the nucleus), and B refers to an effective charge given by (18), which is assumed to minimize the neglected, inhomogeneous, portion of the differential equation defining the Vainshtein function  $g(\mathbf{r}_1, \mathbf{r}_2)$ . The introduction of the effective charge given by (18) into the

present theory decreases the calculated cross sections by about 50% at the peak. However in the Vainshtein version the effective charge shifts the position of the peak and increases its height by 50%. As the introduction of the effective charge reduces the interaction potential between the two electrons it would seem more natural for the effective charge to reduce the cross section.

The only difference between the present theory and that of Vainshtein et al. is that Vainshtein arbitrarily introduces a change of sign in (20) while we evaluate (20) exactly. Figure 2 shows that it is this sign change which is most important in causing the agreement between the theory of Vainshtein et al. and the experimental data of Fite and Brackmann<sup>19</sup> in the  $1s \rightarrow c$  transition. The effect of this approximation is even greater in the  $2s \rightarrow c$  and  $2p \rightarrow c$  cases as is shown in Figs. 3-4. The only reason given by Vainshtein et al. for making this change of sign is that the peaking approximation should over-estimate the cross sections and the sign change will tend to compensate for this. The peaking approximation has recently been shown to give very poor results in two other scattering theories<sup>20,21</sup> but there seems to be no definite criteria for judging the accuracy of the peaking approximation in a given case. The only known check is to do the integral exactly. In the Vainshtein theory the authors are attempting to do this by numerical integration, however it appears to be a formidable task. Until this integration is completed, both the peaking approximation and the sign change should be considered of doubtful validity.

It should be mentioned that Crothers and McCarroll<sup>22</sup> got around Vainshtein's sign change in (20) by using the Post matrix element for the transition amplitude. Their results for excitation cross sections were much closer to Vainshtein et al.'s, than to those given without the change of sign approximation. While Crothers<sup>11</sup> has published details of how the Crothers-McCarroll approximation could be applied to ionization, no ionization cross sections have yet been published for this method.

No numerical calculations using the exchange formulae (25), (28) and (29) are given in this paper as we thought the peaking approximations made should first receive further study.

### C. Comparison of Theories

In Figs. 5-7 the B.E. (i) and B.E. (ii) are compared with the first Born approximation, with the Born-Ochkur exchange calculations of Prasad<sup>4</sup> and with the original Vainshtein and Vainshtein-exchange formulas (21) and (22), for the transitions  $1s \rightarrow c$ ,  $2s \rightarrow c$ , and  $2p \rightarrow c$  (averaged over  $m = 0, \pm 1$ ). In Fig. 5 the  $1s \rightarrow c$  case is shown. Note that the B.E. (ii) calculation agrees best with the experiment of Fite and Brackmann<sup>19</sup> at low impact energies, but that all the curves excepting only the first Born, are fairly closely grouped. The  $2s \rightarrow c$  and the  $2p \rightarrow c$  cases appear quite different from the ground state. The various exchange theories are no longer closely grouped together, except for the B.E. (ii) and Born-Ochkur exchange approximations which nearly coincide. The B.E. (i) curve has moved up close to the first Born curve while both the Vainshtein and the Vainshtein-exchange curves have dropped far below the others.

For large principle quantum number,  $n$ , the ionization cross section,  $Q$ , should be proportional to  $n^4$  both classically and quantum mechanically. In fact if for large  $n$   $Q/n^4$  is plotted versus the impact energy divided by  $n^2$  the curves for the various  $n$  should coincide. Normally we should expect this to be more or less true for small  $n$ . Comparison of the  $Q(1s \rightarrow c)$  and  $Q(2\ell m \rightarrow c)$  at the peak of the curves in Figs. 5-7 shows that this expectation is fulfilled by all the theories shown except the original Vainshtein theory. Figures 2-4 show that the Vainshtein theory without the change of sign also fails to satisfy the scaling law.

At high impact energies the Vainshtein theory goes to the first Born approximation but it does so more slowly than the other theories mentioned here. At 400 eV there is a small but noticeable difference between the cross sections predicted by the first Born and the Vainshtein theories.

In three of the approximations discussed in this paper exchange has been included in such a way as to automatically reduce the calculated cross sections. These approximations are: the Born-Ochkur Eq. (7), the original Vainshtein theory Eq. (23), and the B.E. (ii) version, Eq. (6), of the Born exchange theory. However the inclusion of exchange can cause the cross sections to increase. Table 1 shows that for the transition  $2p m = \pm 1 \rightarrow c$  our B.E. (i) cross sections are larger than the first Born approximation. The differential cross sections were also increased at certain angles and energies in the  $2s$  and  $2p m = 0$  cases although in these latter cases the integrated cross sections were decreased. The

upper bound of possible cross sections in the Born exchange theory lies as far above the first Born curve as the B. E. (ii) points lie below it.

We would like to acknowledge useful conversations with Dr. M. H. Mittleman about the Binary Collision Theory. All numerical calculations were done on the IBM 360-50-65 of the Laboratory for Theoretical Studies, Goddard Space Flight Center.

## Appendix A

In this appendix we try to justify the use of the effective charge approximation. Since the derivation to the approximation is given neither by Vainshtein et. al nor in an analogous paper by Crothers and McCarroll,<sup>22</sup> it is appropriate that this derivation will be given here.

In finding the form of  $Q$  when  $\rho$  and  $R$  are large we assume that according to (16),  $\chi(R, \rho) = \exp[-i \mathbf{k}_1 \cdot (R + \rho)] g_0(R, \rho)$ . Then by making use of the asymptotic form of the confluent hypergeometric functions we can show that

$$\nabla_\rho \ln \chi \underset{\rho \rightarrow \infty}{\sim} \frac{i\nu}{\rho} \left[ \hat{\mathbf{a}}_\rho + \frac{\sin \theta'}{1 - \cos \theta'} \hat{\mathbf{a}}_{\theta'} \right] [1 - e^{z'} - 2i\nu \ln(-iz') + 2i\gamma], \quad (\text{A1})$$

$$\nabla_R \ln \chi \underset{R \rightarrow \infty}{\sim} \frac{i\nu}{R} \left[ \hat{\mathbf{a}}_R + \frac{\sin \theta''}{1 - \cos \theta''} \hat{\mathbf{a}}_{\theta''} \right] [1 - e^{z''} + 2i\nu \ln(-iz'') - 2i\gamma], \quad (\text{A2})$$

where  $\theta'$  and  $\theta''$  are angles of colatitudes of  $\rho$  and  $R$  with respect to  $\mathbf{k}_1$  as the  $z$ -axis, and  $\hat{\mathbf{a}}_\rho$  and  $\hat{\mathbf{a}}_{\theta'}$  are unit vectors in the directions that  $\rho$  and  $\theta'$  increase. Similar definition applies to  $\hat{\mathbf{a}}_R$  and  $\hat{\mathbf{a}}_{\theta''}$ . Similarly

$$z' = i k_1 \rho (1 - \cos \theta'), \quad z'' = i k_1 R (1 - \cos \theta''), \quad \gamma = \arg \Gamma(1 + i\nu) \quad (\text{A3})$$

For atomic states we have analogously

$$\nabla \ln \varphi(1s) = -\alpha_1 \hat{\mathbf{a}}_r, \quad (\text{A4})$$

$$\nabla \ln \varphi(2s) = -\alpha_2 \left( \frac{2 - \alpha_2 r}{1 - \alpha_2 r} \right) \hat{\mathbf{a}}_r, \quad (\text{A5})$$

$$\nabla \ell_n \varphi (2p_m = 0) = \left( \frac{1}{r} - \alpha_2 \right) \hat{\mathbf{a}}_r - \frac{\hat{\mathbf{a}}_\theta}{r} \tan \theta, \quad (\text{A6})$$

$$\nabla \ell_n \varphi (2p_m = \pm 1) = \left( \frac{1}{r} - \alpha_2 \right) \hat{\mathbf{a}}_r + \frac{\hat{\mathbf{a}}_\theta}{r} \cot \theta \pm \frac{i \hat{\mathbf{a}}_\varphi}{r \sin \theta}. \quad (\text{A7})$$

In these equations  $\alpha_1 = Z/a_0$  and  $\alpha_2 = Z/2a_0$ , with  $Z$  the nuclear charge and  $a_0$  the Bohr radius.  $\hat{\mathbf{a}}_1$ ,  $\hat{\mathbf{a}}_\theta$ , and  $\hat{\mathbf{a}}_\varphi$  are unit vectors for the spherical coordinates  $r, \theta, \varphi$ .

For  $\rho$  and  $R$  large the second terms in the second brackets of (A1) are rapidly oscillating functions with unit magnitude. If we neglect them, we get for the 1s case

$$\nabla \ell_n \varphi (1s) \cdot \nabla_\rho \ell_n \chi \sim \frac{i\nu\sqrt{2\epsilon_1}}{\rho} \left[ \cos \theta - \frac{\sin \theta \sin \theta'}{1 - \cos \theta'} \right] \quad (\text{A8})$$

$$\nabla \ell_n \varphi (1s) \cdot \nabla_R \ell_n \chi \sim \frac{-i\nu\sqrt{2\epsilon_1}}{\rho} \left[ \cos \theta - \frac{\sin \theta \sin \theta''}{1 - \cos \theta''} \right] \quad (\text{A9})$$

If we neglect the angular part in the bracket of (A8), we can say that the absolute value of  $\nabla \ell_n \varphi (1s) \cdot \nabla_\rho \ell_n \chi$  cancels the  $(1 - \zeta)/\rho$  term in (16) provided we take  $1 - \zeta = \nu\sqrt{2\epsilon_1}$ . This will then lead to (18). However, in reaching this conclusion, we have (i) replaced  $g(\mathbf{R}, \rho)$  by  $g_0(\mathbf{R}, \rho)$ , (ii) considered only the region  $\rho \rightarrow \infty$ , (iii) neglected the angular factor in (A8), and (iv) taken the absolute value of the gradient term. The validity of these approximations is questionable.

For the 2s and the 2p,  $m = 0, \pm 1$  states Eq. (18) similarly holds with  $\epsilon_1$ , the ionization potential for these states provided we consider the region  $r_1 \rightarrow \infty$ . This



latter approximation makes the effective change approximation even less valid for the excited states. These considerations apply also to the Crothers and McCarroll's paper (Ref. 22), where the gradient terms contain the excited states.

While it is difficult to estimate the accuracy of the effective change approximation, it is found that cross sections are sensitive to variations in the effective change.

## Appendix B

This appendix shows the failure of the peaking approximation when applied to the core term of the direct matrix element in the binary collision theory of Vainshtein. To obtain the Vainshtein core term, (15) and (17) are substituted into the matrix element (2), and the following Fourier transforms are introduced

$$\varphi_2^*(\mathbf{r}_1) \varphi_1(\mathbf{r}_1) = \int \tilde{\varphi}(\mathbf{p}_1) e^{-i\mathbf{p}_1 \cdot \mathbf{r}_1} d^3 p_1, \quad (\text{A10})$$

$$\frac{1}{r_2} = \frac{1}{2\pi^2} \int \frac{1}{p_2^2} e^{i\mathbf{p}_2 \cdot \mathbf{r}_2} d^3 p_2. \quad (\text{A11})$$

The core term becomes

$$\begin{aligned} T^c(1, 2) &= - \langle \varphi_2(\mathbf{r}_1) e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \left| \frac{1}{r_2} \right| \varphi_1(\mathbf{r}_1) g_0(\mathbf{R}, \boldsymbol{\rho}) \rangle \\ &= -8N(2\pi)^{-7/2} \int \frac{d^3 s_1 d^3 s_2 \tilde{\varphi}\left(\frac{\mathbf{s}_1 - \mathbf{s}_2}{2}\right)}{(\mathbf{s}_1 - \mathbf{s}_2 - 2\mathbf{q})^2} \\ &\quad \times \int e^{i\mathbf{R} \cdot \mathbf{s}_1} F(i\nu, 1, i\mathbf{k}_1 \mathbf{R} - i\mathbf{k}_1 \cdot \mathbf{R}) d^3 \mathbf{R} \\ &\quad \times \int e^{i\boldsymbol{\rho} \cdot \mathbf{s}_2} F(-i\nu, 1, i\mathbf{k}_1 \boldsymbol{\rho} - i\mathbf{k}_1 \cdot \boldsymbol{\rho}) d^3 \boldsymbol{\rho}, \end{aligned} \quad (\text{A12})$$

where

$$\mathbf{s}_1 = \mathbf{p}_2 + \mathbf{p}_1 + \mathbf{q}, \quad \mathbf{s}_2 = \mathbf{p}_2 - \mathbf{p}_1 + \mathbf{q}, \quad \mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2. \quad (\text{A13})$$

Following Vainshtein et al., we now make a peaking approximation in (A12). The integral with respect to  $\mathbf{R}$  increases without limit as  $s_1 \rightarrow 0$  while the integral with respect to  $\boldsymbol{\rho}$  increases without limit as  $s_2 \rightarrow 0$ . But notice that when

$s_1 = s_2 = 0$  that  $\tilde{\varphi}(0) = 0$ . Thus when part of the integrand becomes very large another part becomes very small and therefore we cannot apply the peaking approximation.

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Table I

## Born Exchange Cross Sections

The Born exchange and the first Born cross sections, in units of  $\pi a_0^2$ , are given here as calculated by four dimensional numerical quadrature. The Born exchange cross sections B.E. (i) and B.E. (ii) refer respectively to the phase choices given in Eqs. (5) and (6).

Energy	<u>(2s <math>\rightarrow</math> c)</u>		<u>(2pm = 0 <math>\rightarrow</math> c)</u>		<u>(2pm = <math>\pm 1 \rightarrow</math> c)</u>		<u>Average (2p <math>\rightarrow</math> c)</u>	
	<u>Born</u>	<u>B.E. (i)</u>	<u>B.E. (ii)</u>	<u>Born</u>	<u>B.E. (i)</u>	<u>B.E. (ii)</u>	<u>Born</u>	<u>B.E. (i) B.E. (ii)</u>
Ryd.	<u>Born</u>	<u>B.E. (i)</u>	<u>B.E. (ii)</u>	<u>Born</u>	<u>B.E. (i)</u>	<u>B.E. (ii)</u>	<u>Born</u>	<u>B.E. (i) B.E. (ii)</u>
0.36	10.70	9.813	6.784	9.390	7.748	6.139	10.73	10.83 6.323 10.29 9.803 6.262
0.64	17.65	16.27	12.45	20.96	16.74	15.12	19.13	20.24 12.57 19.71 19.07 13.42
1.0	16.02	15.11	12.16	20.57	17.19	15.88	17.35	18.75 12.50 18.42 18.23 13.62
1.44	13.31	12.73	10.46	17.34	15.24	14.14	14.14	15.27 10.93 15.21 15.26 12.00
3.24	7.47	7.25	6.60	9.52	9.08	8.56	7.53	7.91 6.54 8.19 8.30 7.21

## FIGURE CAPTIONS

Fig. 1. The fixed coordinate system  $(x, y, z)$  and the variable system  $(x', y', z')$  used in the Born exchange calculation. The transition amplitude, (8), is evaluated in the  $(x', y', z')$  system, but it must then be transformed to the  $(x, y, z)$  system to allow the interference cross section, (13), to be evaluated. The Eulerian angles relating the two systems are  $\Theta$ ,  $\Phi$  and  $\Psi$ . In this problem  $\Psi$  is arbitrary so we set it equal to zero by choosing  $x'$  perpendicular to  $k_1$ . The polar and azimuthal angles of  $k$  are  $(\alpha, \beta)$  in the  $(x, y, z)$  system and  $(\alpha', \beta')$  in the primed system. The transforms of the spherical coordinates from the unprimed to the primed system are given by Goldstein (Ref. 15).

Fig. 2. Ionization of H(1s). Study of the effective charge and the change of sign approximations in the Vainshtein binary collision theory. The experimental curve is from Fite and Brachmann (Ref. 19). The non-exchange theoretical curves 1A and 1B come from the Vainshtein et al. version, Eq. (21), of the binary collision approximation, while 2A and 2B come from the Omidvar version, Eq. (19) and (22), of this approximation. A refers to an effective charge of unity (no screening by the nucleus), and B refers to an effective charge given by Eq. (18).

Fig. 3. Ionization of H(2s) by electron impact. The labels on the curves have the same meaning as in Fig. 2. Note that this is a log-log plot and cross sections less than one are not shown.



Fig. 4. Ionization of H(2p). Cross sections are averaged over  $m = 0, \pm 1$ . The labels on the curves have the same meaning as in Fig. 2.

Fig. 5. Cross sections for the ionization of H(1s) by electron impact. The experimental curve is from Fite and Brachmann (Ref. 17). The Born exchange cross sections B.E. (i) and B.E. (ii) refer to Eqs. (4-6) and the Born-Ochkur exchange to Eq. (17). The Vainshtein curves were calculated using formulas (21) and (23) which were taken directly from Vainshtein et. al. (Ref. 8).

Fig. 6. Ionization of H(2s) by electron impact. The labels on the curves have the same meaning as in Fig. 5.

Fig. 7. Cross sections for the ionization of H(2p) averaged over ( $m = 0, \pm 1$ ). The labels on the curves have the same meaning as in Fig. 5.

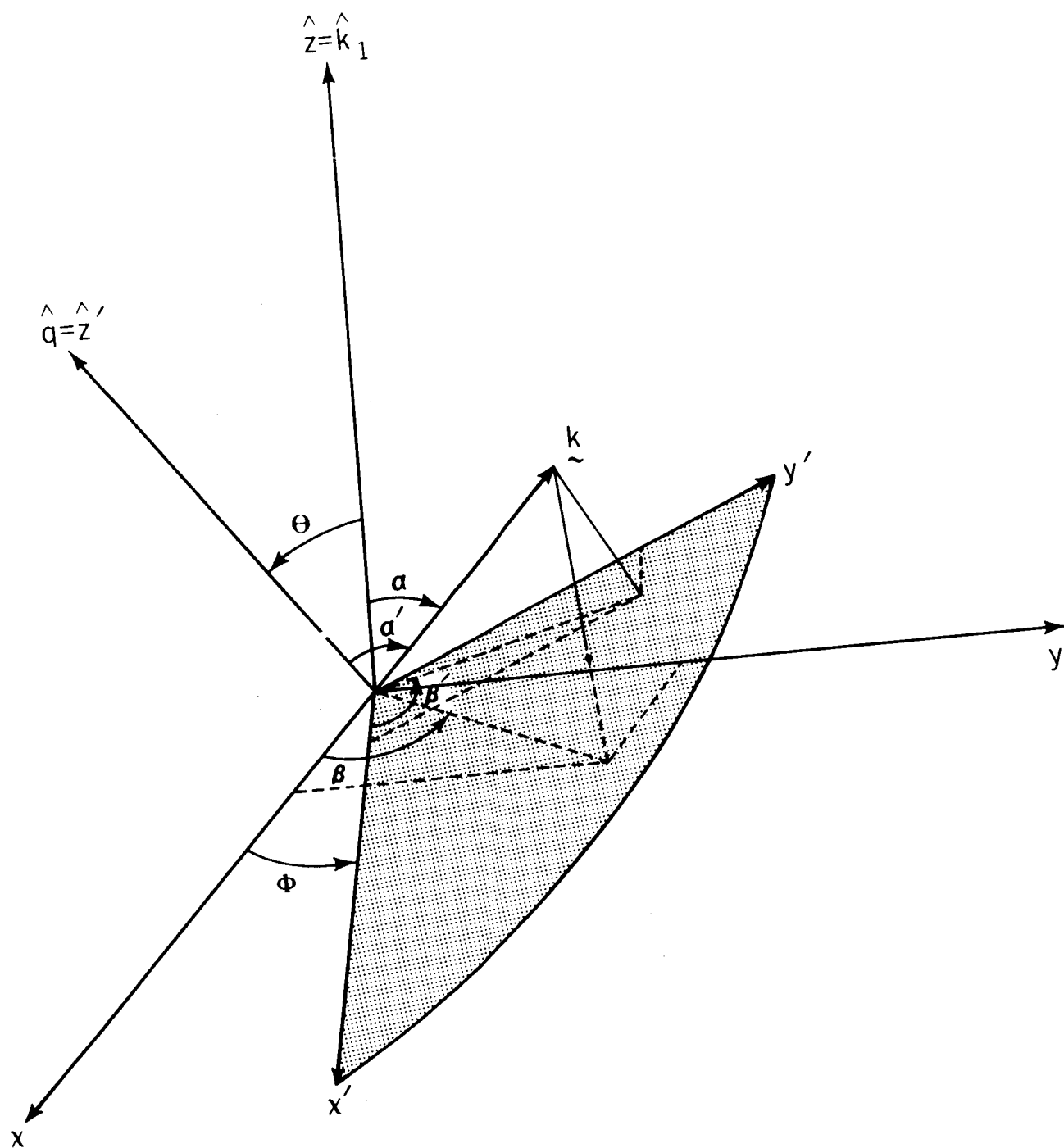


Fig. 1

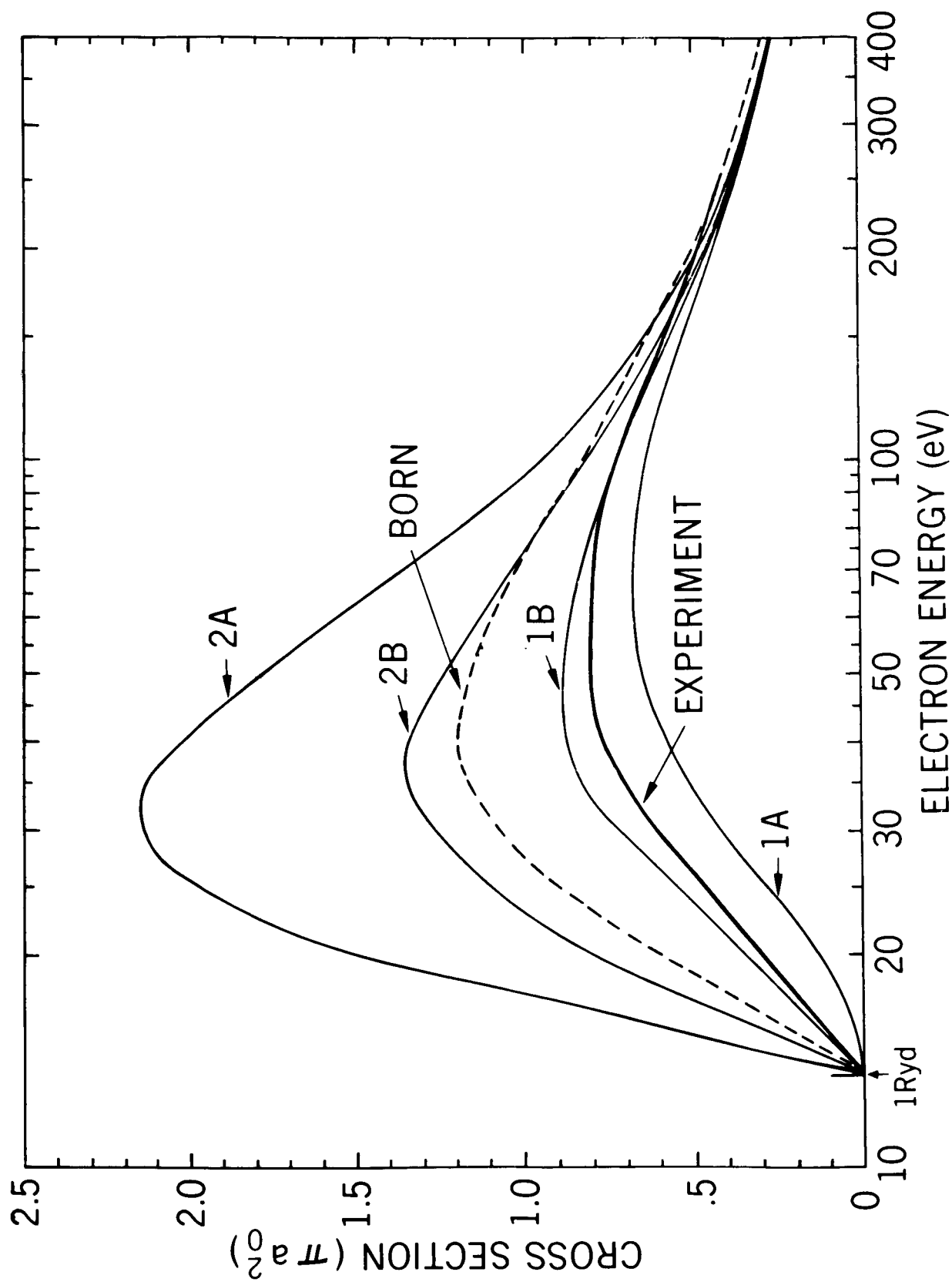


Fig. 2

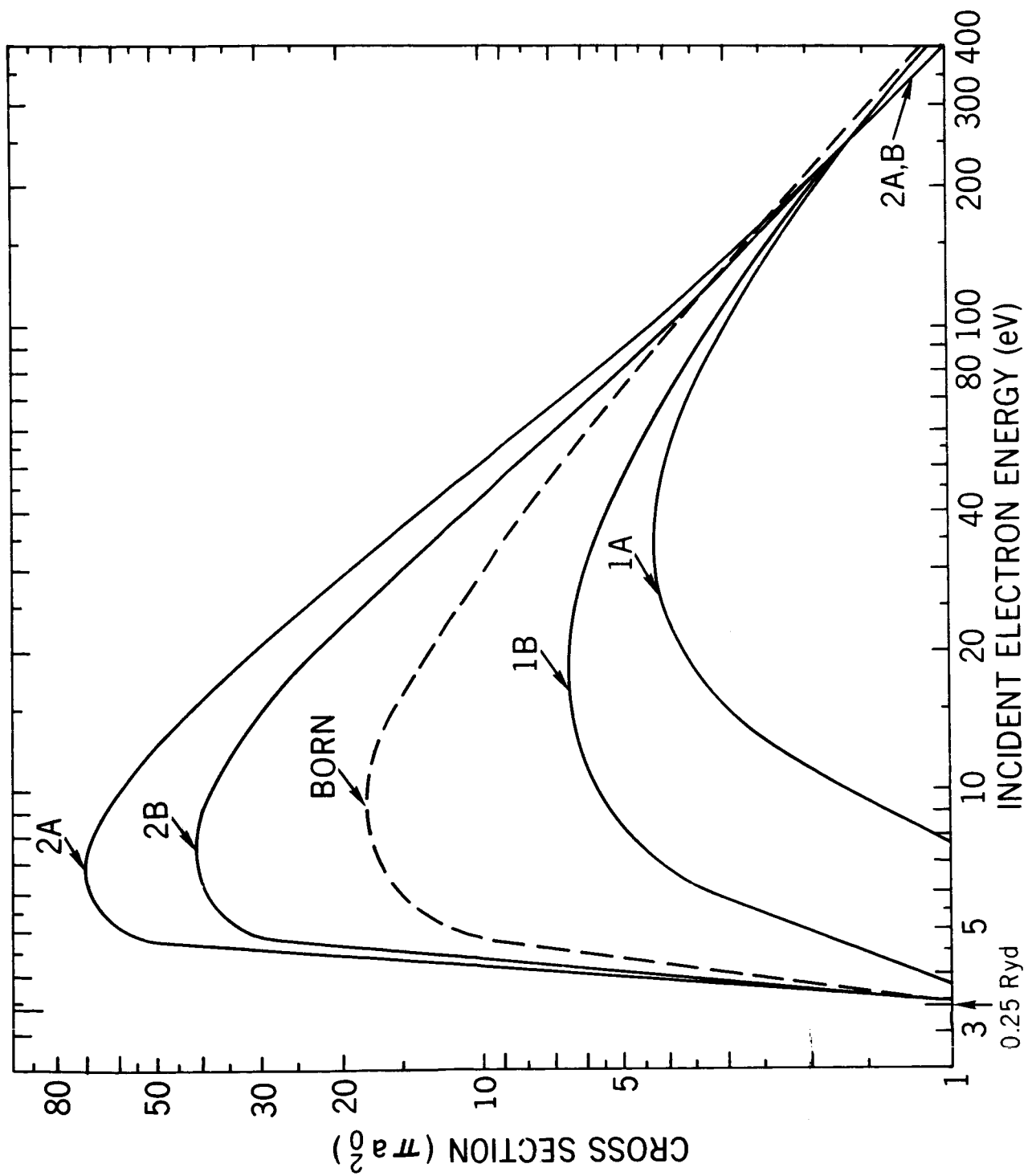


Fig. 3

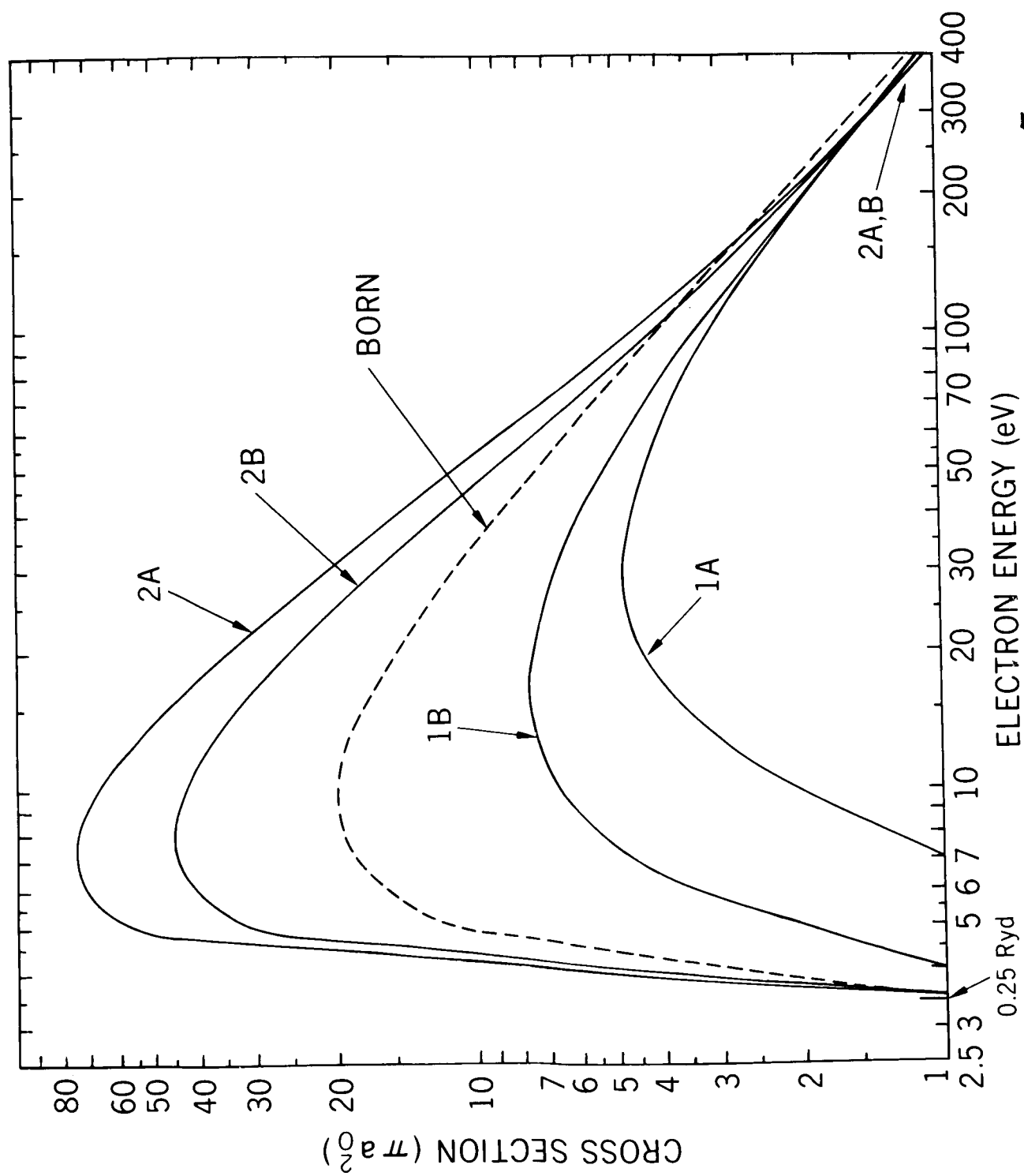


Fig. 4

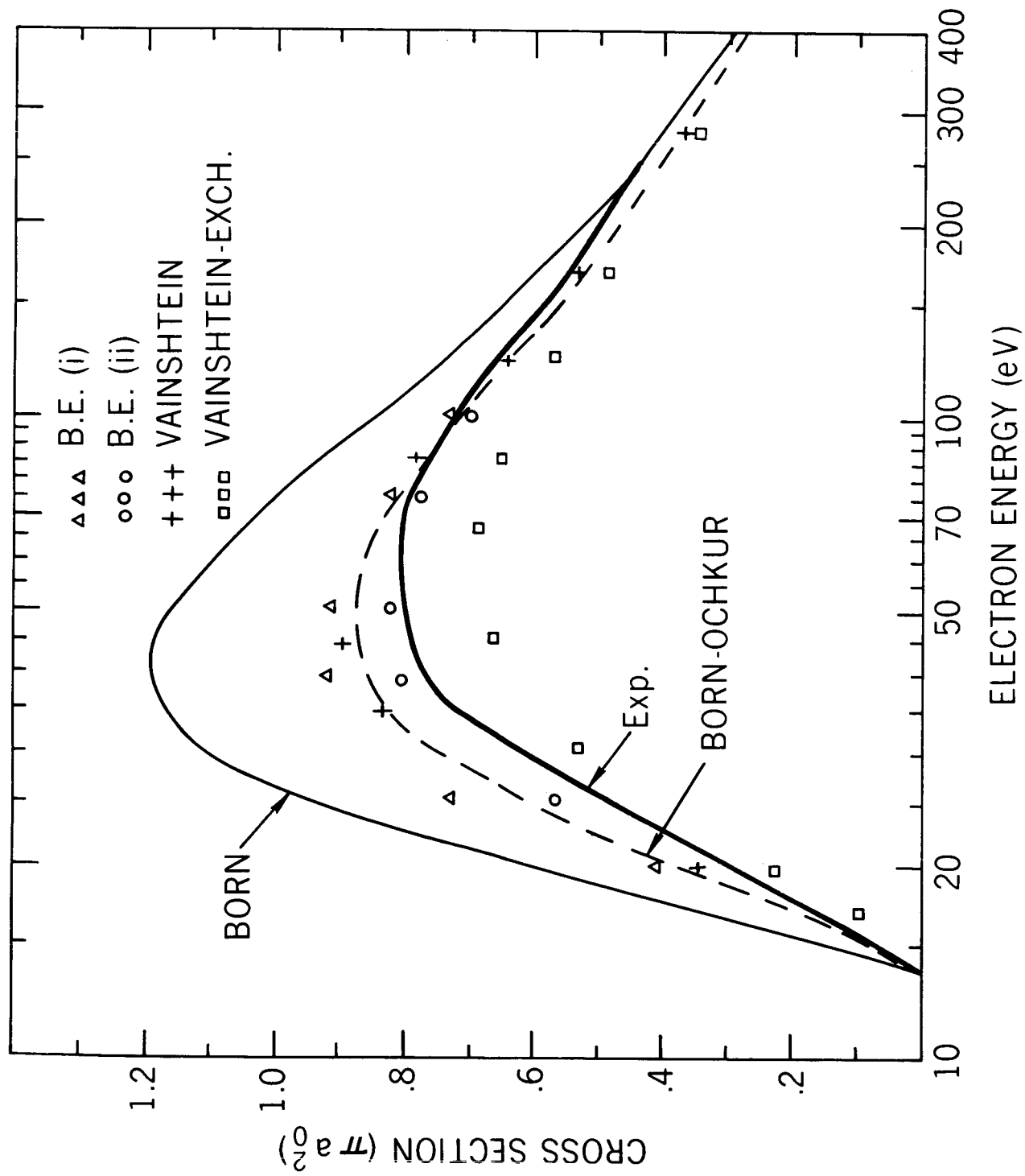


Fig. 5

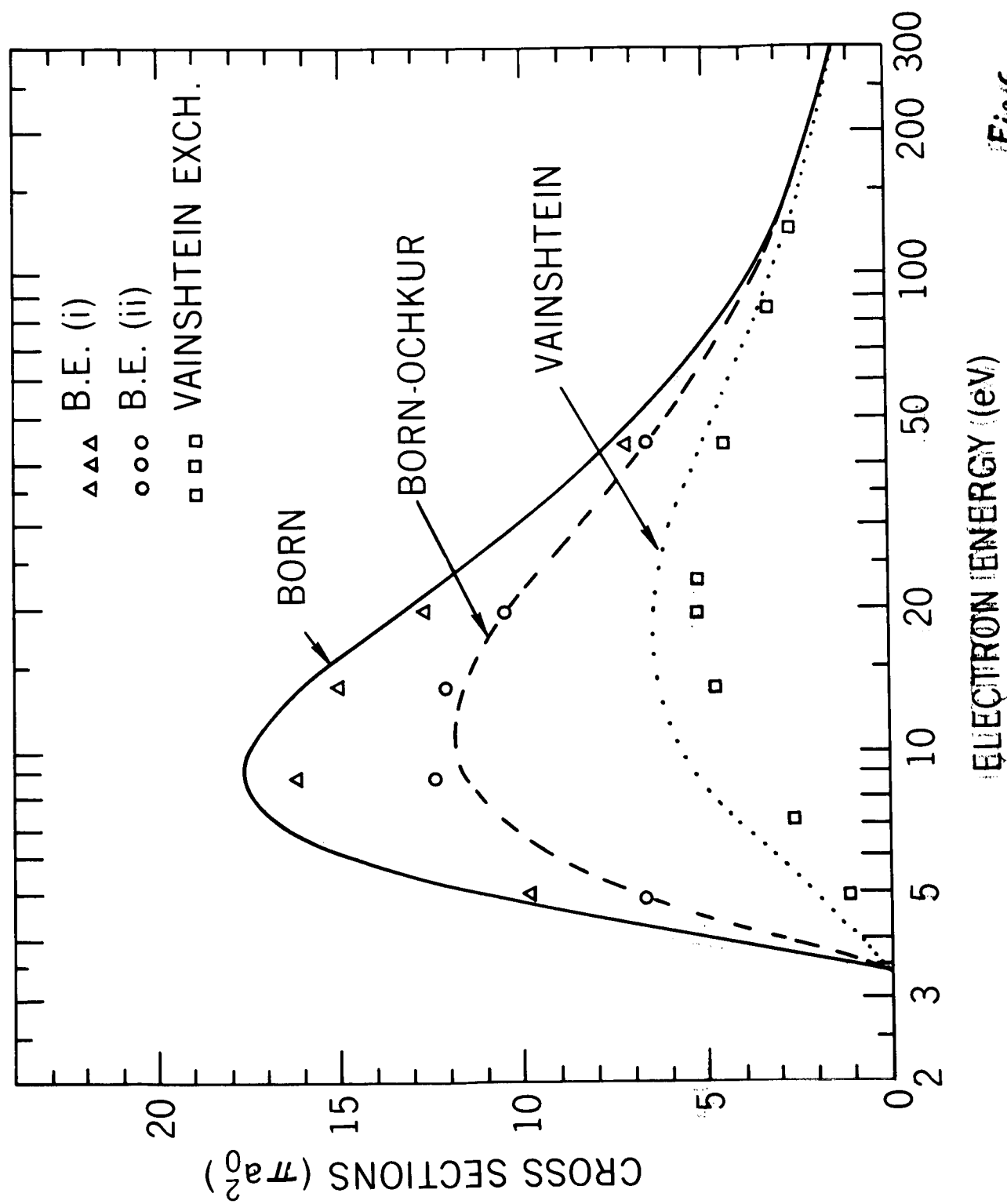


Fig. 6

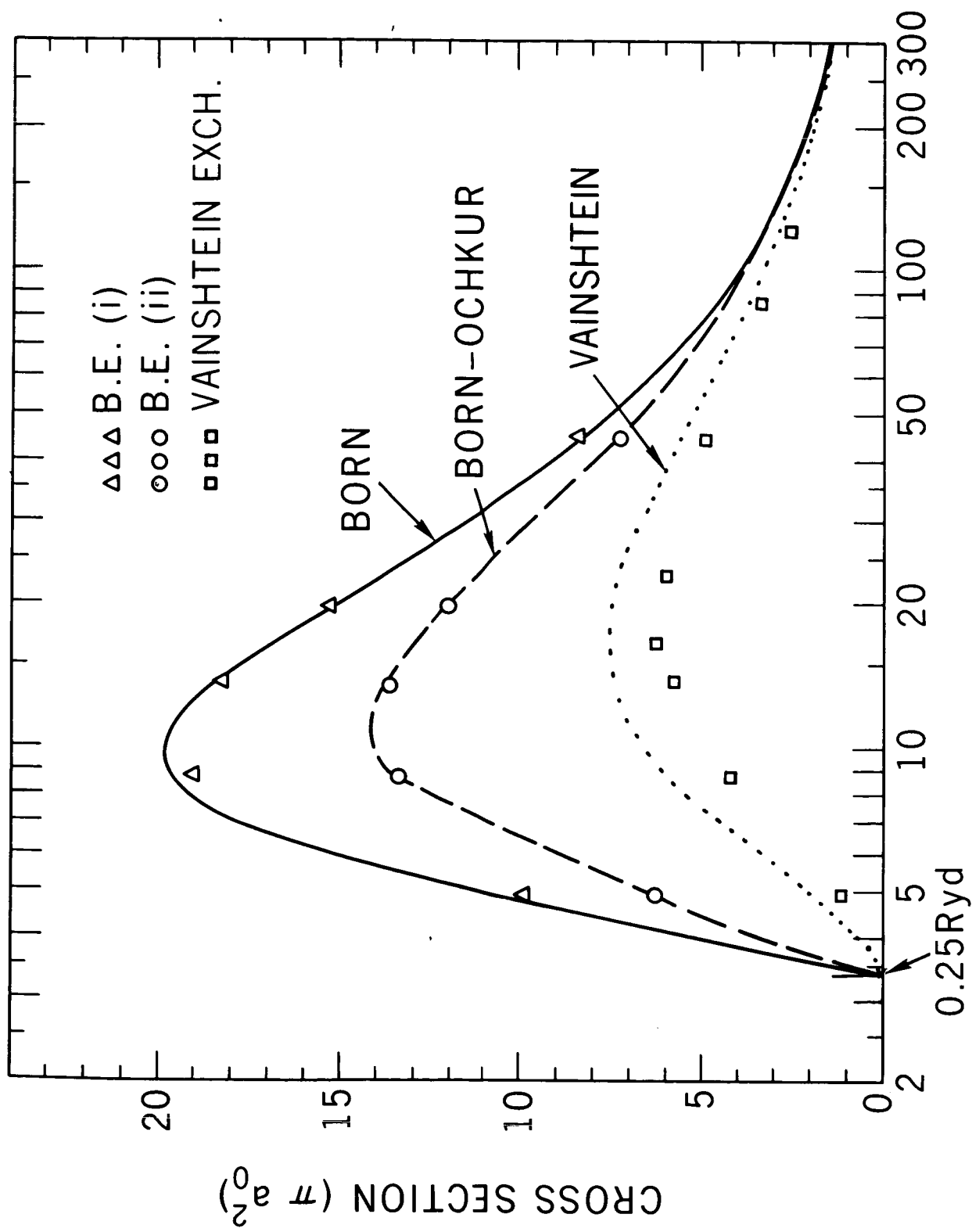


Fig. 7